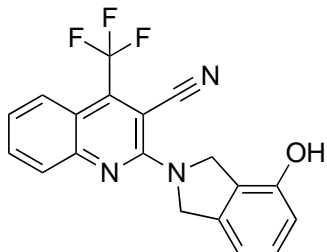


READDI-AC Compound CV

Compound IDs

Investigator or Origin	DENV2 Green site Virtual screening
Investigator ID	Kostya Popov
READDI-AC ID	RA-0003301-01
SMILES	<chem>OC=1C=CC=C2CN(CC21)C=3N=C4C=CC=CC4=C(C3C#N)C(F)(F)F</chem>

Hit properties:



Viral Family	Flavivirus	Notes
Target	NS5 (RdRp)	
Site	Green	
Gel-based Assay (DENV2 RdRp)		Inhibition (100 μM)
Gel-based Assay (LASV RdRp)		Inhibition (100 μM)
In-vitro Potency (DENV2, RdRp)	3.2	μM (IC ₅₀) Gel-based assay
Gel-based Assay (h-mtRNAP)		Inhibition (100 μM)
In-vitro Binding (CGI)	16	μM (Kd) Binding
Anti-viral activity DENV2	3.4	μM (EC ₅₀)
Anti-viral activity DENV4	4.1	μM (EC ₅₀)
MW	355	
cLogP		
Ligand Efficiency		
PSA		A ²
Permeability/ Efflux Ratio		Papp x 10 ⁶ (cm/sec)
Solubility	1.33	μM